

Dimensional crossover of transport characteristics in topological insulator nanofilms

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We show how the two-dimensional (2D) topological insulator evolves, by stacking, into a strong or weak topological insulator with different topological indices, proposing a new conjecture that goes beyond an intuitive picture of the crossover from quantum spin Hall to the weak topological insulator. Studying the conductance under different boundary conditions, we demonstrate the existence of two conduction regimes in which conduction happens through either surface- or edge-conduction channels. We show that the two conduction regimes are complementary and exclusive. Conductance maps in the presence and absence of disorder are introduced, together with 2D \mathbb{Z}_2 -index maps, describing the dimensional crossover of the conductance from the 2D to the 3D limit. Stacking layers is an effective way to invert the gap, an alternative to controlling the strength of spin-orbit coupling. The emerging quantum spin Hall insulator phase is not restricted to the case of odd numbers of layers.

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I. INTRODUCTION

Three-dimensional (3D) topological insulators (TIs) are classified into strong and weak,^{1–3} depending on the number of gapless (Dirac) points in the surface Brillouin zone. A strong topological insulator (STI) typically exhibits a single Dirac cone that is robust against disorder.^{4–7} The surface state of a weak topological insulator (WTI) with a pair of Dirac cones is superior in controllability, e.g., its transport characteristics are sensitive to nanoscale formations of the sample.⁸

The existence of a topologically protected surface state has been confirmed experimentally by spin-resolved ARPES measurements in a number of STI materials,⁹ and is now firmly established.¹⁰ Recently, a WTI has also been experimentally identified.¹¹ Yet, as for triggering the topological nature of transport characteristics, trials done in 3D bulk systems have been unsuccessful due to the difficulty of separating the bulk and surface contributions in transport quantities.¹² In this sense, experimental observation of the topological nature of transport is still restricted to two dimensions,¹³ and a natural step forward is to extend this 2D result to the case of 3D TI nanofilms.^{14–18} Indeed, the study of TI nanofilms is of great interest recently not only in its original but also in related contexts.^{19–23}

There exists a simple picture of the construction of a WTI in which the WTI is viewed as stacked layers of quantum spin Hall (QSH) states, i.e., “(QSH) ^{N_z} \simeq WTI” in the limit of $N_z \rightarrow \infty$, where N_z is the number of stacked QSH layers.^{21,22,24–27} This is indeed a useful point of view, explaining how the helical edge state of a 2D QSH state evolves into the even number of Dirac cones on the surface of a WTI. Here, we examine how precisely such a point of view can be applied to the description of an actual crossover between the 2D and the 3D limits in TI thin films.^{28–34} An alternative view of the

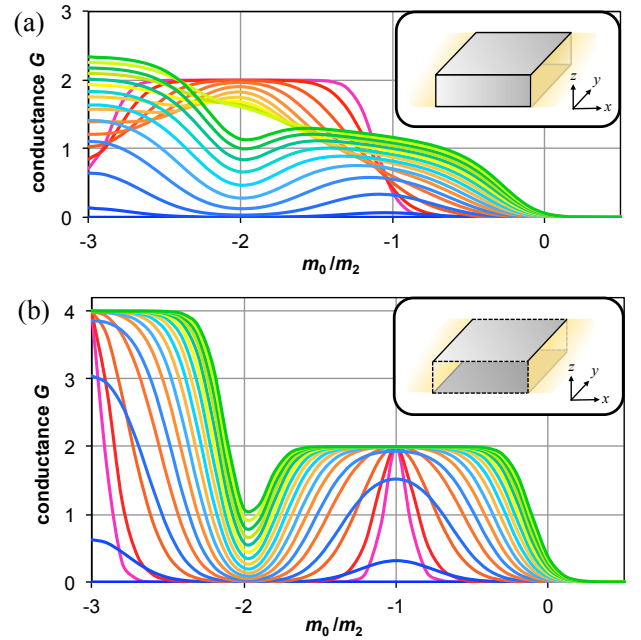


FIG. 1. (Color online) Evolution of the conductance with variation of the film thickness N_z and mass parameters (m_0 and m_2 are defined in Sec. II). Different curves correspond to different N_z values. Two types of boundary conditions [side surfaces are (a) truncated vs (b) periodic] are employed to highlight conduction plateaus of two different origins: edge vs surface conduction. See Sec. III A for a detailed interpretation and settings.

same dimensional crossover is to approach it from the 3D side, i.e., starting with a bulk TI, and making the system thinner and thinner. In this second point of view, evolution of the 3D topological features is attributed to *hybridization* of the top and bottom surface wave functions through the bulk. The first “(QSH) ^{N_z} \simeq WTI” picture

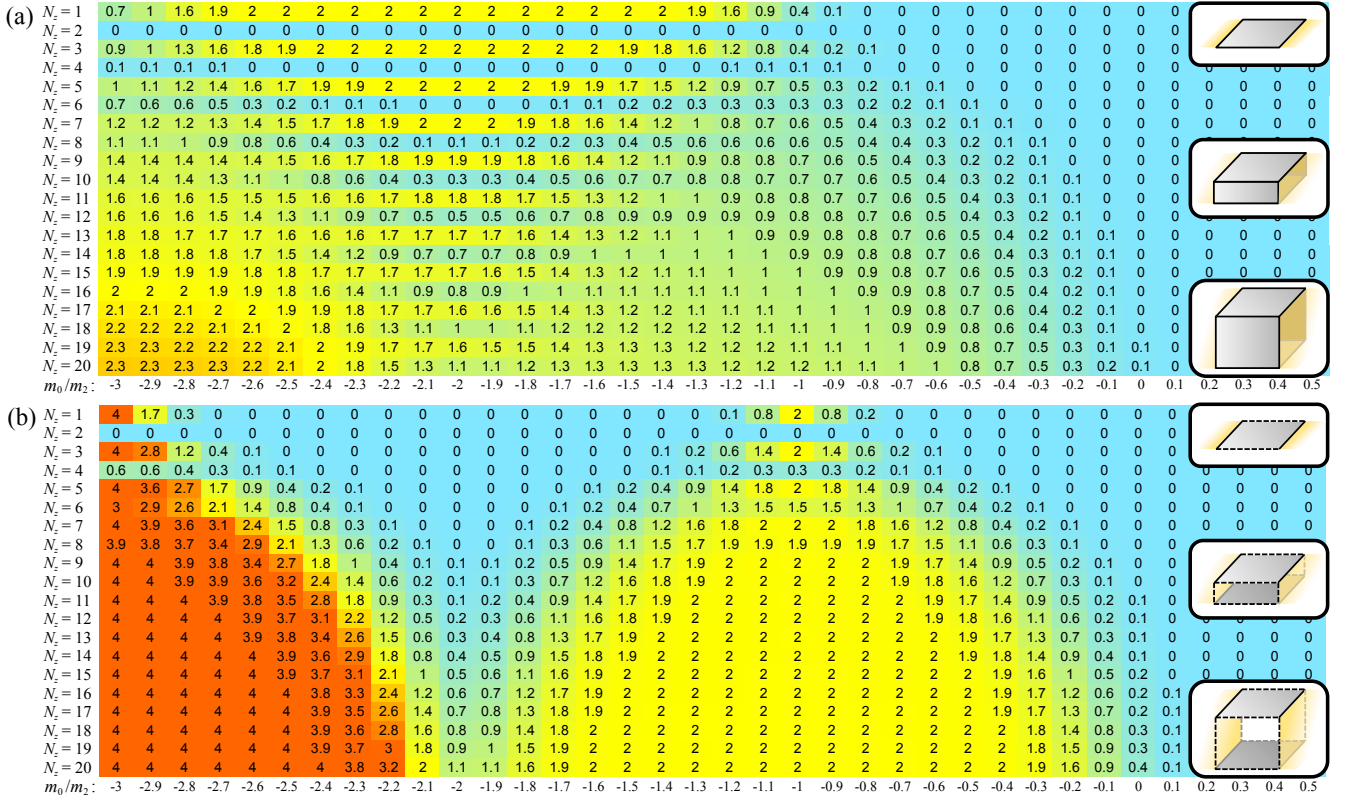


FIG. 2. (Color online) The same conductance data as shown in Fig. 1 are replotted in the form of “conductance maps” to highlight the edge and surface conduction regimes. Numbers listed are conductance values. See Sec. IIIB for a detailed interpretation of the map.

is typically a surface (2D) point of view, while the second picture is, in a sense, a bulk (3D) point of view and applicable in both the STI and the WTI regimes, as long as the surface state wave function extends to the top and bottom surfaces. In this paper we show, by studying the 2D-3D crossover over a broad range of parameters, how the above contrasting (surface- vs bulk-based) points of view compensate each other to give a proper interpretation of the crossover phenomena observed in different parameter regimes, i.e., in different phases (for example, STI vs WTI).

We examine this crossover from the two viewpoints. We first study the conductance of the nanofilm numerically under different boundary conditions: truncated vs periodic in the direction of the width of the film (see Fig. 1). Studying conductance in these two different boundary conditions, we demonstrate the existence of two conduction regimes: *edge* and *surface* conduction regimes, in which conduction happens through either surface or edge conduction channels. The two conductance maps obtained (Fig. 2) show that the two conduction regimes are complementary and exclusive. In order to interpret such conductance maps, we then take the first (2D) viewpoint in which TI thin film is regarded as an effective 2D system, and we calculate 2D \mathbb{Z}_2 indices, introducing \mathbb{Z}_2 -index maps. The \mathbb{Z}_2 -index maps will demonstrate that a 2D ordinary insulating layer is converted to

a TI as identical layers are stacked and coupled; i.e., a nontrivial \mathbb{Z}_2 nature becomes *emergent* by stacking.

The paper is organized as follows. In Sec. II we introduce a standard model Hamiltonian for the description of a bulk TI. Here, the same effective Hamiltonian is used to represent TI thin films by implementing it as a tight-binding model. The main objective of the paper is to interpolate different topological properties in the 2D and 3D limits. By its nature, the 2D or 3D \mathbb{Z}_2 index alone is insufficient for the description of this dimensional crossover. In Sec. III, we overcome this difficulty by studying conductances of TI nanofilms and establish conductance maps as shown in Fig. 2. A sketch of the employed methods and interpretation of the obtained conductance maps are given there. Then in Sec. IV, we attempt to classify such TI thin films of varying layer thicknesses in terms of the 2D \mathbb{Z}_2 indices. We establish the phase diagrams of the thin films as the effective 2D system. Effects of disorder are addressed in Sec. V, before the paper is concluded in Sec. VI.

II. MODEL HAMILTONIAN

Let us start by defining our model Hamiltonian and its parameters. The model Hamiltonian is introduced in the 3D, bulk limit. It turns out to be convenient to

define the bulk Hamiltonian on a lattice, i.e., as a tight-binding Hamiltonian. Here, the type of this lattice is chosen to be *cubic*, and the results of all subsequent analyses are superficially dependent on the choice of this lattice. Then, by truncating this tight-binding Hamiltonian in real space we model a TI nanofilm.

A. Bulk: 3D limit

As a model for a 3D bulk TI, we consider the following Wilson-Dirac model, here implemented as a tight-binding Hamiltonian on a cubic lattice,

$$H_{\text{bulk}}(\mathbf{k}) = m(\mathbf{k})\beta + \sum_{\mu=x,y,z} t_{\mu} \sin k_{\mu} \alpha_{\mu}, \quad (1)$$

where

$$m(\mathbf{k}) = m_0 + \sum_{\mu=x,y,z} m_{2\mu}(1 - \cos k_{\mu}). \quad (2)$$

The length unit is set to the lattice constant. $H(\mathbf{k})$ is a 4×4 matrix, spanned by two types of Pauli matrices $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$, each representing physically real and orbital spins. The explicit form of the Wilson-Dirac Hamiltonian, Eq. (1), corresponds to the choice of α and β matrices such that

$$\alpha_{\mu} = \tau_x \otimes \sigma_{\mu}, \quad \beta = \tau_z \otimes 1_2, \quad (3)$$

where $\mu = x, y, z$. The “Dirac nature” of the Hamiltonian is encoded in the anti-commutation relation of these matrices:

$$\{\alpha_{\mu}, \alpha_{\mu'}\} = 2\delta_{\mu\mu'}, \quad \{\alpha_{\mu}, \beta\} = 0. \quad (4)$$

B. Thin film: An effective 2D system

The tight-binding form of the bulk effective Hamiltonian, Eq. (1), is useful for implementing the thin film geometry. To realize a film of thickness N_z extended in the (x, y) plane, we first rewrite the k_z dependence of Eqs. (1) and (2) in terms of real-space hopping terms, then truncate the hopping outside the system composed of N_z layers starting at $z = 1$ and ending at $z = N_z$. The explicit form of such a tight-binding Hamiltonian reads

$$H_{\text{film}}(k_x, k_y) = 1_{N_z} \otimes \left(m_{2D}^{(k_x, k_y)} \beta + \sum_{\mu=x,y} t_{\mu} \sin k_{\mu} \alpha_{\mu} \right) + H_z, \quad (5)$$

where

$$m_{2D}^{(k_x, k_y)} = \left(m_0 + m_{2z} + \sum_{\mu=x,y} m_{2\mu}(1 - \cos k_{\mu}) \right), \quad (6)$$

and

$$H_z = \begin{pmatrix} 0 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{pmatrix} \otimes \left(-\frac{m_{2z}}{2} \beta \right) + \begin{pmatrix} 0 & -1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & 1 & 0 \end{pmatrix} \otimes \left(i \frac{t_z}{2} \alpha_z \right). \quad (7)$$

Here, the first part of the direct products in Eqs. (5) and (7) represent the layer degrees of freedom. This Hamiltonian consists of two types of contributions; the first term of Eq. (5)—we may call it H_{xy} —is composed of diagonal blocks, each corresponding to a different layer and consisting of an effective 2D Hamiltonian in the layer, while the second term, H_z , represents hopping between such layers.

C. Nanofilm case: Study of the dimensional crossover

Since the main interest in this paper is the study of a dimensional crossover between 2D and 3D limits, we employ TI nanofilms with their boundaries truncated in all three spatial directions, i.e., finite-sized samples. Considering TI nanofilms, we found it useful to rewrite Hamiltonian (1) in real space as

$$H = \sum_{\mathbf{x}} \sum_{\mu=x,y,z} \left(\frac{it_{\mu}}{2} c_{\mathbf{x}+\mathbf{e}_{\mu}}^{\dagger} \alpha_{\mu} c_{\mathbf{x}} - \frac{m_{2\mu}}{2} c_{\mathbf{x}+\mathbf{e}_{\mu}}^{\dagger} \beta c_{\mathbf{x}} + \text{h.c.} \right) + (m_0 + m_{2x} + m_{2y} + m_{2z}) \sum_{\mathbf{x}} c_{\mathbf{x}}^{\dagger} \beta c_{\mathbf{x}}, \quad (8)$$

where \mathbf{x} is a position of lattice sites and \mathbf{e}_{μ} is the lattice vector in the μ direction.

III. CONDUCTANCE MAP

Using the model Hamiltonian, Eq. (8), introduced in the previous section, we study the conductance of TI nanofilms numerically. Studying the conductance under different boundary conditions (recall Fig. 1), we demonstrate the existence of two conduction regimes: the *edge* and *surface conduction* regimes. To reveal the nature of these two conduction regimes, especially with regard to its thickness dependence, the same data as shown in Fig. 1 are replotted in Fig. 2 in a different format: as conductance maps.

A. Numerical study of conductance

We focus on the two terminal conductance G of TI nanofilms, hereafter measured in units of e^2/h , and at

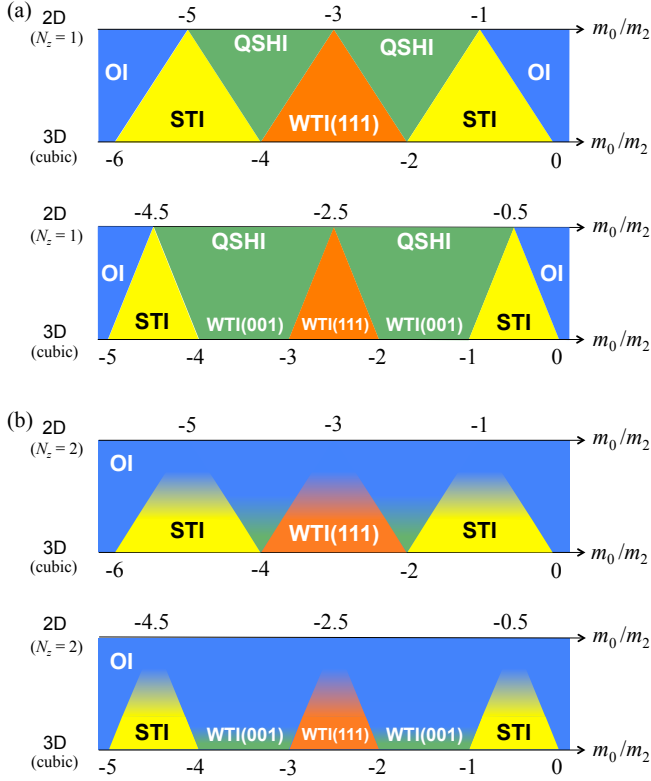


FIG. 3. (Color online) Phase diagram: an abstracted form of the conductance map. Comparison of the cases of (a) N_z odd and (b) N_z even. Comparison of the isotropic (upper panel) vs anisotropic (lower panel) cases; see Eqs. (9) and (12). Valid in the regime of $|t_z/m_{2z}| > 1$. The edge (surface) conduction regimes are represented as green (yellow/red) areas.

Fermi energy $E = 0$. Using the transfer matrix method,⁶ we calculate the transmission coefficients for each conduction channel, then deduce the two-terminal conductance G with the help of the Landauer formula.

To study the behavior of G , we employ the geometry shown in the insets in Fig. 1. We also employ two types of boundary conditions, truncated vs periodic, in the direction of the width of the film (y direction), corresponding to a film with vs without edges, respectively. Here, we have placed the sample in such a way that the film is on the xy plane, while leads are attached to the two extremities of the sample in the x direction; i.e., the conduction occurs in the x direction. The leads consist of 1D perfectly conducting channels, so that the effect of the leads is minimized.

Figure 1 shows typical examples of our conductance data. In both panels, the two-terminal conductance G is plotted as a function of m_0/m_2 ; i.e., the evolution of the conductance with the change of the mass parameter m_0 introduced in Eq. (2). Here, the mass parameters m_{2x} , m_{2y} and m_{2z} are chosen to be isotropic:

$$m_{2x} = m_{2y} = m_{2z} = m_2. \quad (9)$$

We have also set the strength of hopping t_z such that $t_z/m_{2z} = 2$. Different curves in Fig. 1 correspond to

different thicknesses N_z of the film. The size of the system is such that the top and bottom surfaces are of size $L_x \times L_y = 20 \times 20$, while the thickness N_z of the film is varied from 1 to 20. Reddish curves, to the case of N_z odd; bluish curves correspond to the case of N_z even; while greenish curves, to cases where N_z is so large that the system looks like a cubic geometry rather than a film.

In the 2D limit, i.e., at $N_z = 1$, the system is either in the QSH phase [$\nu_0^{2D} = 1$, see Eq. (13) for definition] with a pair of helical edge modes, or in the ordinary insulator (OI) phase ($\nu_0^{2D} = 0$) without an edge mode, depending on the value of m_0/m_2 . The QSH phase occurs in the range $-3 < m_0/m_2 < -1$, while the OI phase corresponds to $-1 < m_0/m_2$. The QSH phase implies a plateau of the conductance at $G = 2$ in the truncated geometry [Fig. 1(a)], while $G = 0$ is expected in the OI phase. Such a tendency can be seen in the reddish curves in Fig. 1(a). Note that in this truncated geometry the contribution from the edge conduction channels is accentuated.

However, in the 3D limit or, more practically, in the cubic geometry $N_z = L_x = L_y$, the phase boundaries between topologically different phases are shifted from the above 2D values. The system is expected to be in the STI phase in the range $-2 < m_0/m_2 < 0$, while it is in the WTI phase with weak indices $\nu^{3D} = (111)$ at $-4 < m_0/m_2 < -2$. The OI phase corresponds to $0 < m_0/m_2$. Let us focus on Fig. 1(b), the case of periodic boundary conditions. In this geometry, the film has no edge so that only contributions from the top and bottom surfaces are well maintained, as long as the bulk is gapped and insulating. In the STI phase the existence of a single Dirac cone on the top and bottom surfaces implies a conductance plateau at $G = 2$, while in the WTI phase double Dirac cones on the top and bottom surfaces sum up to $G = 4$. One can see a precursor of such plateaus in the greenish curves in Fig. 1(b).

B. The conductance map

We have so far seen that the Figs. 1(a) and 1(b) indeed show conductance plateaus of two different natures: the edge and surface conduction types. They also appear in different parameter regimes, so that there are edge and surface conduction regimes. In Fig. 2 we have replotted the same data as shown in Fig. 1 in a different format, as “conductance maps”, to reveal the nature of these two conduction regimes. Presented in this way, the existence of two conduction regimes may become apparent.

1. Edge vs surface conduction regimes

The nature of the two conductance plateaus is apparent in Figs. 2(a) and 2(b). The conductance plateaus at $G = 2$ associated with the edge conduction channels that appear in the regime of m_0/m_2 centered at

$m_0/m_2 = -2$ in Fig. 1(a) are arranged into the vertically striped, downward-pointing triangle region at the left in Fig. 2(a): the *edge conduction regime*. Such conductance plateaus are shown by the reddish curves in Fig. 1(a), i.e., at an odd number of layers, while the bluish curves, i.e., at an even number of layers, show vanishing conductance in the same range of m_0/m_2 ; therefore, an alternating pattern of $G = 2$ and $G = 0$ is shown in the conductance map in Fig. 2(a). Note that in the conductance map the vertical axis represents the film thickness N_z , encoding the dimensional crossover of transport characteristics.

Similarly, the conductance plateaus at $G = 2$ and at $G = 4$ in Fig. 1(b) form the two upward-pointing triangular regions in Fig. 2(b), corresponding to STI and WTI regimes. Naturally, such conduction plateaus are associated with bulk conduction channels, so they can be seen as the greenish curves in Fig. 1(b). In Fig. 2(b), the two corresponding triangular regions become predominant in the limit of large N_z . As N_z is decreased, a region of vanishing conductance appears between the two triangular regions, which corresponds, in the parameter space of $(m_0/m_2, N_z)$, to the edge-conduction regime in Fig. 2(a).

Quantized conduction in TI nanofilms is caused by either the surface, or the edge conducting channels. The two types of conducting channels are not completely open at the same time. Only one of the channels is always open except in the crossover regime, in which both channels are partially open. The two conduction regimes are, therefore, both *complementary* and *exclusive*. Away from the 2D or 3D limits, at which transport characteristics are simply determined by the 2D or 3D \mathbb{Z}_2 topological indices, the conductance maps cast a new perspective on the competitive nature of 2D TI-like (edge conduction) and 3D TI-like (surface conduction) properties.

2. Surface point of view: Approach from the 2D limit

In the 2D limit, i.e., at $N_z = 1$, the QSH phase occurs in the range of parameters $-3 < m_0/m_2 < -1$. A plateau of the quantized conductance at $G = 2$ appears in this parameter regime, due to the pair of helical edge modes circulating around the gapped 2D bulk area. Stacking such a layer in the z direction, one can construct a TI nanofilm with helical edge modes circulating around the side surfaces. When N_z layers are stacked, N_z pairs of helical edge modes are incident on the side surfaces and couple with each other. If N_z is even, they are all gapped, while if N_z is odd, there always exists a single combination that remains gapless and perfectly conducting even in the presence of disorder. The origin of the striped pattern in the edge-conduction regime in Fig. 2(a) is this even/odd feature.

In the above picture the helical edge modes circulating around the side surfaces are expected to become an even number of Dirac cones characteristic of a WTI surface, while the top and bottom surfaces are kept gapped. This situation is realized in a WTI state with weak indices

$\nu^{3D} = (001)$, and this indeed happens in the case of the standard “(QSH) $N_z \simeq$ WTI” picture. However, the situation we have here is slightly different. In the 3D limit of our system, a WTI phase is indeed expected in the range of parameters $-4 < m_0/m_2 < -2$, but its weak indices are $\nu^{3D} = (111)$; i.e., the top and the bottom surfaces are *not* gapped in this phase. Also, an STI phase is expected in the range of parameters $-2 < m_0/m_2 < 0$. In the 2D-3D crossover shown in the conductance maps in Fig. 2, there is no WTI state expected from the 2D side as a consequence of the standard “(QSH) $N_z \simeq$ WTI” crossover. In Fig. 2(a) the region showing a striped pattern indeed becomes narrower as N_z is increased toward the line of $m_0/m_2 = -2$.

What, then, happens in our 2D-3D crossover regime? Actually, what can be regarded as a WTI state with weak indices $\nu^{3D} = (001)$ is uncoupled layers of QSH states stacked in the z direction, which corresponds in the present context to the limit of

$$m_{2\perp} = m_{2z} = 0. \quad (10)$$

The phase diagram of our model Hamiltonian, (1), in the 3D limit in the case of such an anisotropic choice of parameters can be found in Fig. 1 in Ref. 26, where

$$m_{2\parallel} = m_{2x} = m_{2y}. \quad (11)$$

One notes in that phase diagram that the $m_{2\perp} = 0$ line in this 3D phase diagram is nothing but the 2D limit we have already considered; only the QSH phase is replaced by a WTI state with weak indices $\nu^{3D} = (001)$. Starting with this limit and switching on $m_{2\perp}$ adiabatically, one can follow the evolution of the system from this 2D limit to an isotropic line, $m_{2\perp} = m_{2\parallel}$, which we regard here as the 3D limit. The STI phase and the WTI phase with weak indices $\nu^{3D} = (111)$ emerge and replace the WTI (001) phase as $m_{2\perp}/m_{2\parallel}$ is switched on and approaches unity. A similar phase diagram, consisting of cross-dimensional topological regions, has been proposed recently in the context of cold atoms.²⁰ This is indeed, at least theoretically, a reasonable way to achieve the 2D-3D crossover. Yet, “physically” a more natural way to induce that crossover is to stack layers. Stacking layers is, however, not a continuous deformation, since the number of layers can be changed only discretely. A number of different topological phases emerge as an increasing number of layers is stacked. As the even/odd feature is washed out with increasing N_z in Fig. 2(a), quantized conductance appears as a new emergent feature in the two triangular regions in Fig. 2(b), i.e., in the surface-conduction regimes.

We performed a conductance study also in such an anisotropic regime of parameters, and here we show the results only schematically. In Fig. 3 we divide the information from the conductance map into cases of N_z odd [Fig. 3(a)] and N_z even [Fig. 3(b)], then abstract it into the form of a schematic phase diagram. The upper panels in Figs. 3(a) and 3(b) correspond to the case of an

isotropic choice of parameters, Eq. (9), while the lower panels represent the anisotropic case:

$$m_{2\perp} = m_{2\parallel}/2. \quad (12)$$

In the figure $m_{2\parallel}$ is simply represented as m_2 . On the anisotropic line, Eq. (12), there indeed exists a range of parameters, $-2 < m_0/m_2 < -1$, in which “(QSH) N_z ” leads to an expected WTI with $\nu^{3D} = (001)$.

3. Bulk point of view : Approach from the 3D limit

The film geometry of an STI in the shows “pseudo gapless” surface states in both the top and the bottom surfaces of the film. Here, what we imply by the quotation marks is that usually the surface states are slightly gapped due to hybridization between the top and the bottom surface states. The corresponding wave function has an exponentially decaying tail into the bulk, and the magnitude of the hybridization gap³³ is essentially determined by the remaining amplitude at the opposite surface, i.e., $\psi_{z=N_z}$ of the top surface wave function. As a result, surface conduction is suppressed with decreasing N_z , while in the cubic (3D) case on the bottom low in Fig. 2(b), the hybridization between the top and the bottom surfaces can be neglected.

In the 3D limit, the STI phase is extended over $-2 < m_0/m_2 < 0$. The penetration of such a surface state becomes deeper as one approaches the 3D topological phase boundary at $m_0/m_2 = 0, -2$ (where the Dirac semimetal phase appears). Near the 3D phase boundary, as one reduces the number of layers N_z , a hybridization gap is formed more easily, driving the system to the edge conduction regime at relatively large N_z . With decreasing N_z , quantization of the conductance due to the surface Dirac cones is naturally destroyed, while at the center of the STI phase at $m_0/m_2 = -1$ the surface conduction survives exceptionally down to the single-layer (2D) geometry: $N_z = 1$. This is because at $m_0/m_2 = -1$, the matrix elements between surface states on the top and bottom surfaces vanish and the hybridization gap does not open as long as N_z is odd.

4. Breakdown of the even/odd feature

Figure 4 shows the evolution of conductance in a system with isotropic hopping at $t_z/m_{2z} = 0.5$ with varying film thicknesses under the truncated boundary condition as in Fig. 1(a). The behavior of the conductance in Fig. 4 looks much more irregular compared with that in Fig. 1(a). One can observe that the evolution of the even/odd striped pattern as in Fig. 2(a) remains in the downward-pointing triangular region around $m_0/m_2 = -2$. Outside this region, new plateaus are observed beyond the parameter range where the film becomes a QSHI in the 2D limit ($N_z = 1$), in contrast

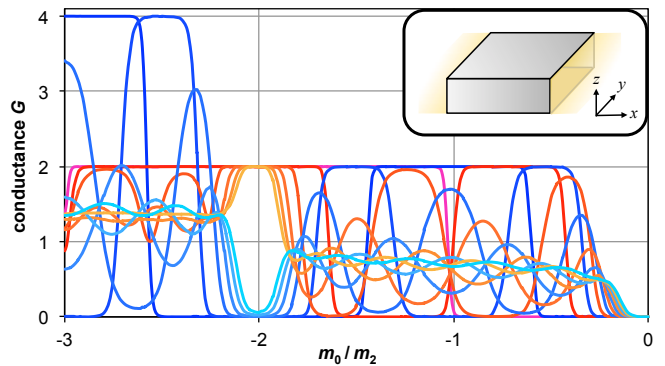


FIG. 4. (Color online) Conductance of TI nanofilms as in Fig. 1(a), but with $t_z/m_{2z} = 0.5$. In contrast to Fig. 1(a), the behavior of the conductance looks rather erratic. The corresponding conductance map is given in Fig. 5(b).

to Fig. 2(a). We note that the emergent plateaus arise even with an *even* number of layers. The breakdown of the even/odd feature occurs in specific parameter regimes that are specified by the analytics in effective 2D systems [see Eq. (33)] and is expected to come from emergent 2D topological phases.

IV. THE \mathbb{Z}_2 INDEX MAP

In contrast to the case of a 3D bulk TI, Eq. (1), a TI thin film, Eq. (5), can be regarded as an effective 2D system, to which 2D topological classification is applied. As a consequence, the phase diagram of the thin film acquires a richer structure, which depends on the thickness of the film.

A. Two-dimensional \mathbb{Z}_2 indices for thin film

A thin film, or a system with slab geometry of finite thickness, is regarded as an effective 2D system. Actually it does not have to be thin, as long as the area of the film is infinite, because the features associated with the motion in the direction of the thickness of the film can be regarded as those of an internal degree of freedom. Here, we take this view and consider Eq. (5) to be an effective 2D bulk Hamiltonian for this quasi-2D system.

Topological classification of gapped free fermionic insulating phases, which physically mean either an insulating or a superconducting phase, is here applied to our thin-film model. The periodic table of TIs and superconductors^{35–37} for the 10 universality classes³⁸ tells us which type of topological invariant can be used to characterize our system, i.e., whether \mathbb{Z} - or \mathbb{Z}_2 -type. The underlying bulk 3D TI of our thin-film model is prescribed by Eq. (1) in the clean limit and belongs to class DIII. However, since we are more concerned about features robust against disorder, we here assume that on-site disorder is implicit in our thin-film model and, also, in

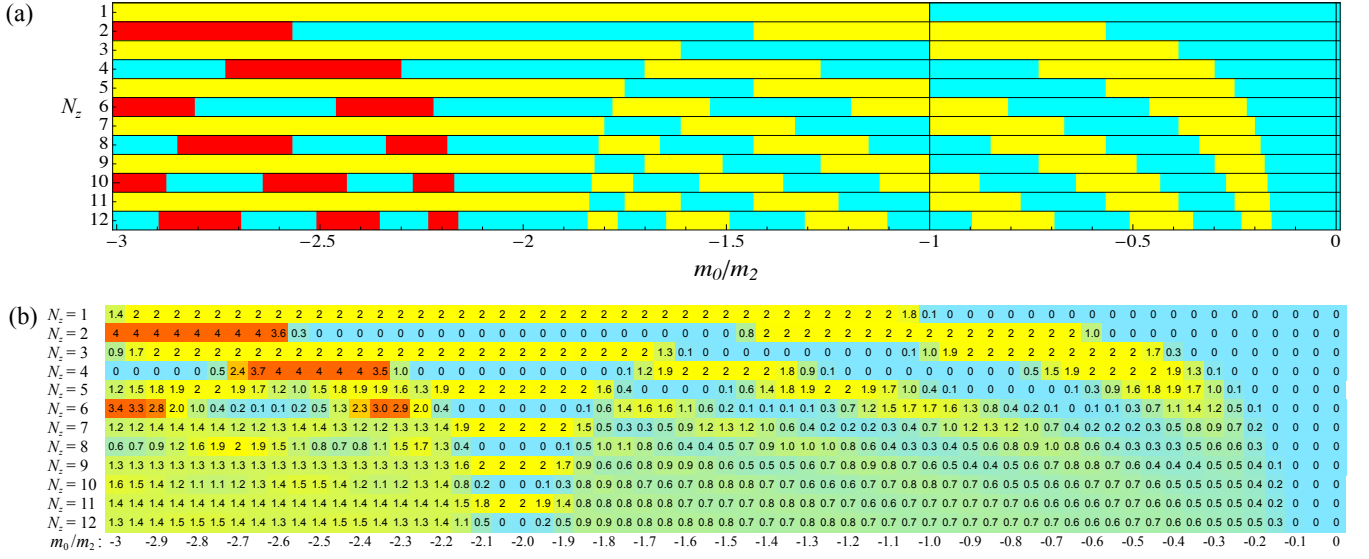


FIG. 5. (Color online) (a) \mathbb{Z}_2 -index map vs (b) conductance map in the case of a relatively small t_z , $t_z/m_{2z} = 0.5$; cf. $t_z/m_{2z} = 2$ in the regime of $t_z > 1$ in Fig. 2. In the regime of relatively small t_z , a stripe pattern prominent in the lower-triangular region in Fig. 2(a) (the edge conduction regime) is extended to a broader range of parameters on the side of smaller $|m_0/m_2|$. But outside the original triangular regime this is no longer an even/odd feature: an effective QSH insulator (QSHI), or 2D TI ($\nu_0^{2D} = 1$) phase (yellow region) appears not just with an odd number of layers. The trivial phase with $\nu_0^{2D} = 0$ corresponds to the blue region, while the red region corresponds to a 2D analog of the more standard 3D weak TI phases.

the parent bulk TI. In the presence of potential disorder, the bulk TI falls into class AII; so does its thin-film analog except in the limit of $N_z = 1$ or $t_z = 0$, where the film Hamiltonian is block diagonalized and each block belongs to class A. The topological classification applicable to a system of symmetry class AII is \mathbb{Z}_2 in both two and three dimensions.

The \mathbb{Z}_2 -topological index ν_0^{2D} is protected by the time-reversal symmetry $\Theta H_{\text{film}}(\mathbf{k})\Theta^{-1} = H_{\text{film}}(-\mathbf{k})$, where $\Theta = -i\beta\alpha_x\alpha_zK$ is the time-reversal operator and K is the complex conjugate operator. Under space inversion symmetry, the \mathbb{Z}_2 -invariants can be written in terms of the parity eigenvalues $\xi_{2m}(\Gamma_i) = \pm 1$ of the occupied bands ($m = 1, 2, \dots, N$) at time-reversal invariant momenta (TRIM) Γ_i ,³⁹ as

$$(-1)^{\nu_0^{2D}} = \prod_{m=1}^{N_z} \xi_{2m}(0,0)\xi_{2m}(\pi,0)\xi_{2m}(0,\pi)\xi_{2m}(\pi,\pi). \quad (13)$$

Here, it is implied that in the Brillouin zone of the 2D square lattice, there are four time-reversal invariant momenta, $\{\Gamma_i\} = \{(0,0), (\pi,0), (0,\pi), (\pi,\pi)\}$, and $2N_z$ of the total $4N_z$ bands are occupied, as long as the Fermi energy is in the gap.

Using eigenstates $|n, \mathbf{k}\rangle$ found explicitly for the model Hamiltonian, Eq. (5), we can determine the parity eigenvalue $\xi_{2m}(\Gamma_i)$ such that

$$P|2m, \mathbf{k} = \Gamma_i\rangle = \xi_{2m}(\Gamma_i)|2m, \mathbf{k} = \Gamma_i\rangle. \quad (14)$$

Note that the $2m$ th and $(2m-1)$ th eigenstates are (Kramers) degenerate, and the Kramers doublet share

the same parity eigenvalue, $\xi_{2m}(\Gamma_i) = \xi_{2m-1}(\Gamma_i)$. Collecting all such parity eigenvalues for (half of) the occupied states, we evaluated the 2D \mathbb{Z}_2 -indices given in Eqs. (13)–(17). Repeating this procedure for different mass parameters and for different number of layers allows for the determination of the phase diagram of a TI thin film. In the evaluation of this formula, it is naturally essential to identify an appropriate inversion operator P that satisfies $PH_{\text{film}}(\mathbf{k})P^{-1} = H_{\text{film}}(-\mathbf{k})$, $P\psi_z(\mathbf{k}) = \psi_{N_z-z+1}(-\mathbf{k})$, and $[P, \Theta] = 0$. In the case of a TI nanofilm, P is given as

$$P = \begin{pmatrix} & & 1 \\ & \ddots & \\ 1 & & \end{pmatrix} \otimes \beta. \quad (15)$$

Clearly, the first part of Eq. (15) plays the role of reversing the layer indices, while the second part reverses the momentum parallel to the film.

In parallel with Eq. (13), it is useful to define the 2D weak indices $\nu^{2D} = (\nu_x^{2D}, \nu_y^{2D})$, as the 2D analog of the more standard 3D weak indices:

$$(-1)^{\nu_x^{2D}} = \prod_{m=1}^{N_z} \xi_{2m}(\pi,0)\xi_{2m}(\pi,\pi), \quad (16)$$

$$(-1)^{\nu_y^{2D}} = \prod_{m=1}^{N_z} \xi_{2m}(0,\pi)\xi_{2m}(\pi,\pi). \quad (17)$$

Similar 2D weak indices have been introduced, e.g., in Ref. 40. These weak indices are associated with chiral symmetry, which manifests on the line $k_x, k_y = 0, \pi$. Dif-

ferent topological sectors are specified by the three topological indices, ν_0^{2D} ; $(\nu_x^{2D} \nu_y^{2D})$.

B. \mathbb{Z}_2 -index map and emergent topological phases

In Fig. 5(a), these 2D \mathbb{Z}_2 topological indices are calculated, varying the gap parameter m_0/m_2 and the thickness N_z , then tabled: this is the “ \mathbb{Z}_2 -index map”. In the map the effective QSHI phase, or a 2D TI phase with ν_0^{2D} ; $(\nu_x^{2D} \nu_y^{2D}) = 1$; (00) or 1; (11), is shown in yellow, the trivial (OI) phase with 0; (00) in blue, and the 2D analog of the 3D WTI phases [0; (11) phase in Fig. 5(a)] in red, to facilitate comparison with the corresponding conductance map [Fig. 5(b)]. Note that the two maps show a reasonably good agreement for small N_z . In Fig. 5(a), the expected even/odd feature of 2D TI states can be seen only for the region around $m_0/m_2 = -2$; outside this region, an effective QSHI, or 2D TI (with $\nu_0^{2D} = 1$) phase (yellow region), appears also at an even number of layers. Yellow bands of the QSHI phase are extended to a broader range of parameters on the side of smaller $|m_0/m_2|$, where the single layer film goes into the OI phase; this implies that a 2D TI phase emerges when OI films are stacked. As a whole, an increasing number of topologically different sectors emerges as the number of layers is increased.

The evolution of the TI and OI phases as a function of N_z demonstrated here represents a feature specific to the case of a relatively small t_z ; in Fig. 5 this is chosen as $t_z/m_{2z} = 0.5$, while the conductance maps shown in Fig. 2 are calculated in the regime of a relatively large t_z ($t_z/m_{2z} = 2$). All of these features do not necessarily manifest in the case of large t_z . The global structure of the phase diagram changes at $|t_z/m_{2z}| = 1$ (see Sec. IV C and the Appendix). In the regime of small t_z as in Fig. 5 the surface-state wave function shows a damped oscillatory behavior into the bulk, while once the hopping exceeds the threshold value $t_z/m_{2z} = 1$, the surface-state wave function is overdamping. Indeed, in the regime of large t_z , $t_z/m_{2z} > 1$, the \mathbb{Z}_2 -index map becomes very simple and we find the calculated \mathbb{Z}_2 -index map not insightful enough to be explicitly shown. By numerical estimations, we have verified that the \mathbb{Z}_2 index ν_0^{2D} in this regime takes the values

$$\nu_0^{2D} = \begin{cases} 1 & (-5 < \frac{m_0}{m_2} < -1 \text{ and } N_z = \text{odd}), \\ 0 & (\text{otherwise}), \end{cases} \quad (18)$$

except for $m_0/m_2 = -5, -3, -1$ with $N_z = \text{odd}$, where \mathbb{Z}_2 index is not well defined (see Sec. IV D).

C. Zeros of the thin film Hamiltonian: A simplified consideration

In the case of the 3D bulk TI of Eq. (1), when the system evolves from a certain TI phase to another, from

an STI to a WTI, with varying model parameters, the bulk energy gap collapses in between. The locus of such a gap closing gives the phase boundaries of the 3D system mentioned in Sec. I. In the case of a TI thin film, the locus of the gap closing of Eq. (5) gives the phase boundary of the 2D system. Although the \mathbb{Z}_2 -index map in the regime of small t_z [Fig. 5(a)] looks complicated compared with the simple behavior in the large- t_z regime, the location of the phase boundaries can be specified systematically in both regimes.

Let us start from the simple case of vanishing t_z . In the limit $t_z \rightarrow 0$, the 2D bulk Hamiltonian, Eq. (5), can be trivially diagonalized, since the inter-layer part of H_z reduces to a matrix of the form

$$\begin{pmatrix} 0 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{pmatrix}. \quad (19)$$

This is diagonalized by a unitary matrix U , and naturally the operation of U and U^{-1} leaves H_{xy} invariant. Physically, each component ψ_z ($z = 1, 2, \dots, N_z$) of the state vector applied to H_z (and also to H_{film} as a whole) is an amplitude of the wave function in the corresponding layer z . Here we choose ψ_z such that $\psi_z = \sin k_z z$ in order to be compatible with the boundary condition $\psi_0 = \psi_{N_z+1} = 0$. This imposes a constraint on the allowed value of k_z such that

$$k_z^{(n)} = \frac{n\pi}{N_z + 1}, \quad (20)$$

where $n = 1, 2, \dots, N_z$. The corresponding eigenvalues of the matrix, Eq. (19) is $2 \cos k_z^{(n)}$, which takes the values: 0 for $N_z = 1$, ± 1 for $N_z = 2$, 0 and $\pm\sqrt{2}$ for $N_z = 3$, etc. Noting that

$$\begin{aligned} & U^{-1} H_{\text{film}}(k_x, k_y) U \\ &= \text{diag} \left[m_{2D}^{(k_x, k_y)} - m_{2z} \cos k_z^{(n=1, \dots, N_z)} \right] \otimes \beta \\ &+ 1_{N_z} \otimes \sum_{\mu=x, y} t_\mu \sin k_\mu \alpha_\mu, \end{aligned} \quad (21)$$

the energies are easily evaluated as

$$\begin{aligned} & E_n(k_x, k_y) \\ &= \pm \sqrt{\left(m_{2D}^{(k_x, k_y)} - m_{2z} \cos k_z^{(n)} \right)^2 + \sum_{\mu=x, y} t_\mu^2 \sin^2 k_\mu}. \end{aligned} \quad (22)$$

Note that at the phase boundary, E_n must vanish at either of the time-reversal symmetric points. At the four symmetric points, the 2D effective Dirac mass takes the following values:

$$\begin{aligned} m_{2D}^{(0,0)} &= m_0 + m_{2z}, \\ m_{2D}^{(\pi,0)} &= m_0 + m_{2z} + 2m_{2x}, \\ m_{2D}^{(0,\pi)} &= m_0 + m_{2z} + 2m_{2y}, \\ m_{2D}^{(\pi,\pi)} &= m_0 + m_{2z} + 2m_{2x} + 2m_{2y}. \end{aligned} \quad (23)$$

In the trivial 2D limit, i.e., the case of $N_z = 1$, the phase transition occurs when $m_{2D}^{(k_x, k_y)} = 0$, i.e., with four values of $m_0 = m_{0c(N_z=1)}^{(k_x, k_y)}$:

$$\begin{aligned} m_{0c(N_z=1)}^{(0,0)} &= -m_{2z}, \\ m_{0c(N_z=1)}^{(\pi,0)} &= -m_{2z} - 2m_{2x}, \\ m_{0c(N_z=1)}^{(0,\pi)} &= -m_{2z} - 2m_{2y}, \\ m_{0c(N_z=1)}^{(\pi,\pi)} &= -m_{2z} - 2m_{2x} - 2m_{2y}. \end{aligned} \quad (24)$$

If Wilson terms are isotropic in the (x, y) plane and denoted

$$m_{2x} = m_{2y} = m_{2\parallel} \neq 0, \quad m_{2z} = m_{2\perp}, \quad (25)$$

then two adjacent parameter regimes (let us call them “QSH regimes”),

$$-\frac{m_{2\perp}}{m_{2\parallel}} - 2 < \frac{m_0}{m_{2\parallel}} < -\frac{m_{2\perp}}{m_{2\parallel}}, \quad (26)$$

$$-\frac{m_{2\perp}}{m_{2\parallel}} - 4 < \frac{m_0}{m_{2\parallel}} < -\frac{m_{2\perp}}{m_{2\parallel}} - 2, \quad (27)$$

separated by a “degenerate” phase boundary, $m_0/m_{2\parallel} = -m_{2\perp}/m_{2\parallel} - 2$, turn out to be twin QSH regimes with a nontrivial spin Chern number, ± 1 . The two QSH regimes belong to a sector of different spin Chern number⁴¹ but they are identical in the \mathbb{Z}_2 classification; both correspond to the $\nu_0^{2D} = 1$ phase.⁴² On the phase boundary $m_0/m_{2\parallel} = -m_{2\perp}/m_{2\parallel} - 2$, two degenerate Dirac cones appear at two distinct time-reversal momenta, $(k_x, k_y) = (\pi, 0)$ and $(0, \pi)$, in the 2D Brillouin zone.

In the case of a bilayer TI nanofilm with $N_z = 2$, the phase boundaries given in the single-layer limit as in Eq. (24) split into two,

$$m_{0c(N_z=2)}^{\Gamma_i} = m_{0c(N_z=1)}^{\Gamma_i} \pm \frac{m_{2\perp}}{2}, \quad (28)$$

as a result of the hopping between layers, described by H_z as given in Eq. (7). The amount of the shift leading to the splitting is determined by the eigenvalue of H_z ; in the present case of $N_z = 2$, it is simply given as ± 1 in units of the prefactor $-m_{2\perp}/2$ of the corresponding hopping term [see Eq. (19) and the text following the equation]. This leads to the pair of transition points around $m_{2\perp}/m_{2\parallel} = -1$ in the $N_z = 2$ row in Fig. 5(a), though in Fig. 5(a) t_z is not 0 but finite, $t_z/m_{2\perp} = 0.5$. In the range sandwiched between two pairs of degenerate gapless points at $(\pi, 0)$ and $(0, \pi)$,

$$-\frac{m_{2\perp}}{m_{2\parallel}} - 2 - \frac{1}{2} \frac{m_{2\perp}}{2m_{2\parallel}} < \frac{m_0}{m_{2\parallel}} < -\frac{m_{2\perp}}{m_{2\parallel}} - 2 + \frac{1}{2} \frac{m_{2\perp}}{2m_{2\parallel}}, \quad (29)$$

a “weak QSHI phase” [see Eqs. (16) and (17)] with two helical edge modes appears: the $G = 4$ region indicated in red [see the $N_z = 2$ row in Fig. 5(b)].

In the case of a trilayer film ($N_z = 3$), similarly to the bilayer case, $m_{0c(N_z=1)}^{\Gamma_i}$ in Eq. (24) split into three as

$$m_{0c(N_z=3)}^{\Gamma_i} = m_{0c(N_z=1)}^{\Gamma_i} + \frac{m_{2\perp}}{2} \times \begin{cases} 0, \\ \pm\sqrt{2}. \end{cases} \quad (30)$$

Note that, in contrast to the case of an even number of layers, in the case of an odd number of layers, H_z always bears a null eigenvalue.

D. Zeros of the thin-film Hamiltonian: A generic case

By generalizing the discussion above to nonzero t_z (see the Appendix), we obtain $4N_z$ gap closing points,

$$\begin{aligned} m_{0c(N_z)}^{(0,0)} &= -m_{2z} + \lambda_n, \\ m_{0c(N_z)}^{(\pi,0)} &= -m_{2z} - 2m_{2x} + \lambda_n, \\ m_{0c(N_z)}^{(0,\pi)} &= -m_{2z} - 2m_{2y} + \lambda_n, \\ m_{0c(N_z)}^{(\pi,\pi)} &= -m_{2z} - 2m_{2x} - 2m_{2y} + \lambda_n, \end{aligned} \quad (31)$$

with

$$\lambda_n = \sqrt{m_{2z}^2 - t_z^2} \cos\left(\frac{n\pi}{N_z + 1}\right), \quad (n = 1, \dots, N_z). \quad (32)$$

The gapped states of the 2D square lattice are classified into $2^4 = 16$ topologically distinct phases⁴⁰ and the gapless points correspond to a boundary between those topologically distinct phases (not necessarily a TI-OI transition).

Examples ($N_z = 3, 4$) of the evolution of the phase diagram with respect to t_z are shown in Fig. 6. As shown in there, the behavior of the phase diagram changes drastically at $|t_z/m_{2z}| = 1$, which is implied in Eq. (31). In the regime of large t_z , $|t_z/m_{2z}| > 1$, only four of the $m_{0c}(\cos k_z^{(n)} = 0, \text{ for } n = \frac{N_z+1}{2})$ are real, and the 2D topological phase boundaries are the same as those of $N_z = 1$, Eq. (24), for $N_z = \text{odd}$ and always trivial ($\cos k_z^{(n)} \neq 0$, for all n) for $N_z = \text{even}$. As a consequence, only the even-odd feature of the QSH regime [see Eqs. (26) and (27)] is persistent. In the regime of small t_z , $|t_z/m_{2z}| < 1$, an increasing number of gapless points (or topologically distinct sectors) emerges as an increasing number of layers is stacked, in the range

$$m_{0c(N_z=1)}^{\Gamma_i} - \sqrt{m_{2z}^2 - t_z^2} < m_0 < m_{0c(N_z=1)}^{\Gamma_i} + \sqrt{m_{2z}^2 - t_z^2}. \quad (33)$$

In contrast to the continuous deformation of the Hamiltonian (e.g., switching off the inter-layer coupling²⁶), stacking the layer can lead to emergent topological phenomena; topologically trivial 2D systems can be driven into 2D TIs by just stacking layers [see, for example, around $m_0/m_2 = -0.5$ in Fig. 5(a)].

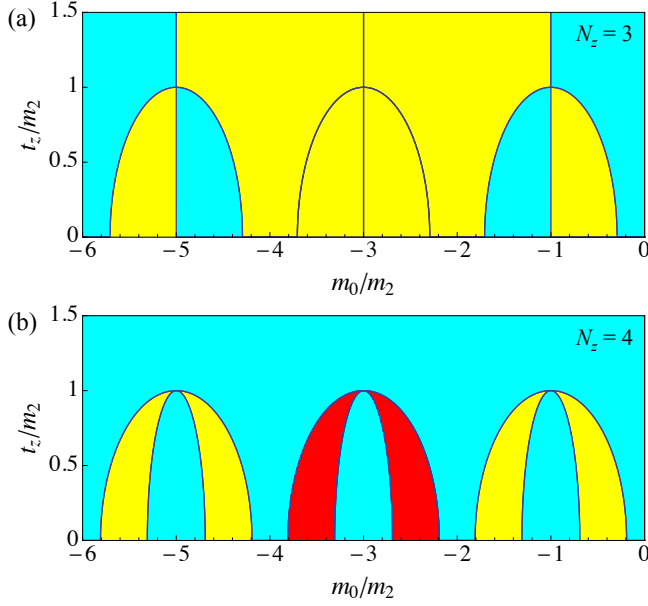


FIG. 6. (Color online) Evolution of the 2D \mathbb{Z}_2 indices of isotropic film ($m_{2x} = m_{2y} = m_{2z} = m_2$) as a function of t_z/m_{2z} . The film thickness is (a) $N_z = 3$ and (b) $N_z = 4$. Solid lines are the zeros of the 2D bulk energy gap specified by Eq. (31), derived in the Appendix, and they correspond to 2D topological phase boundaries. Colors have the same meaning as in Fig. 5, and the intersection of the phase diagram at $t_z/m_{2z} = 0.5$ corresponds to the $N_z = 3$ or $N_z = 4$ row in Fig. 5(a).

We mention that even in the limit $N_z \rightarrow \infty$, the 2D topological phase boundaries do not converge to the 3D phase boundaries (in the case of Figs. 2 and 5, the 3D WTI/STI boundary is located at $m_0/m_2 = -2$ and the 3D STI/OI boundary at $m_0/m_2 = 0$). This is not an inconsistency, however, since the 2D and 3D \mathbb{Z}_2 invariants are different by definition. The bulk of a TI thin film can always, i.e., irrespective of the number of layers, be regarded as an effective 2D system and characterized by 2D \mathbb{Z}_2 invariants, while 3D \mathbb{Z}_2 invariants cannot be defined in the film Hamiltonian, Eq. (5). Although we have revealed a rich structure of emergent topological phases in TI thin films as 2D TIs, we found it difficult to reach the 3D limit and to investigate the dimensional crossover behavior in our thin-film model.

Mapping onto the conductance map Fig. 5(b), one may intuitively expect that its erratic behavior comes from the emergent topological phases as a 2D TI. At $N_z = 2$ in Fig. 5(b), the conductance jumps to a quantized value $G = 2$ in the range $-1.4 \lesssim m_0/m_2 \lesssim -0.6$, while for a large t_z it is *a priori* supposed to vanish [conductance “valley”; see Fig. 2(a)]. Similarly, on the other side, around $m_0/m_2 \lesssim -2.6$ it is again quantized at $G = 4$. The border between the original conductance valley and the new plateau is located at the zeros of the film Hamiltonian, Eq. (5), $m_0/m_2 = -1 \pm \sqrt{3}/4$, $-3 + \sqrt{3}/4$ [see Eq. (31)]. On the contrary, at $N_z = 3$ the conductance is

a priori quantized at $G = 2$, while this original plateau is replaced by a new valley around $-1.6 \lesssim m_0/m_2$, then reappears, forming a new plateau in the range $-0.95 \lesssim m_0/m_2 \lesssim -0.45$. The borders between the two plateaus and the new valley are again given by Eq. (31), $m_0/m_2 = -1$, $-1 \pm \sqrt{6}/4$.

What are the origins of these new valleys and plateaus? In the parameter regime, Eq. (33), the surface wave function is oscillatory,²⁶ and the precise behavior of the damped oscillation continuously varies as a function of the mass parameter. Thus, with changing m_0/m_2 , it happens that $\psi_{z=N_z}$ vanishes at a critical value of m_0/m_2 , then changes sign; correspondingly, the hybridization gap vanishes, then gets *inverted*. In the regime of this inverted hybridization gap, edge states appear just as in the usual QSHI phase.

V. EFFECTS OF DISORDER

The behavior of the conductance in the presence of disorder is an interesting issue to study. Now we examine how robust the features are that we have so far established to be characteristic of the conductance maps in the clean limit. We introduce the on-site random potential of the box distribution $v_{\mathbf{x}} = [-\frac{W}{2}, \frac{W}{2}]$ into Eq. (8),

$$H = \sum_{\mathbf{x}} \sum_{\mu} \left(\frac{it_{\mu}}{2} c_{\mathbf{x}+\mathbf{e}_{\mu}}^{\dagger} \alpha_{\mu} c_{\mathbf{x}} - \frac{m_{2\mu}}{2} c_{\mathbf{x}+\mathbf{e}_{\mu}}^{\dagger} \beta c_{\mathbf{x}} + \text{h.c.} \right) + \left(m_0 + \sum_{\mu} m_{2\mu} \right) \sum_{\mathbf{x}} c_{\mathbf{x}}^{\dagger} \beta c_{\mathbf{x}} + \sum_{\mathbf{x}} v_{\mathbf{x}} c_{\mathbf{x}}^{\dagger} 1_4 c_{\mathbf{x}}, \quad (34)$$

where the summation of μ runs over x, y, z . Figures 7(a) and 7(b) are conductance maps under two boundary conditions analogous to those in Fig. 2, but in the presence of on-site disorder $W = 3$. One can see that the addition of disorder leads to effects associated with the so-called “topological Anderson insulators”, i.e., the emergence of nontrivial topological characters upon the addition of disorder.^{43,44} This is a feature due to renormalization of the Dirac mass, which eventually changes its sign when the strength of disorder attains a certain critical value.^{44,45} In Fig. 7 this appears as a shift of phase boundaries in comparison with those in Fig. 2. However, one can also confirm there that, apart from this shift, the addition of disorder does not lead to a dramatic effect on the features of conductance maps in the clean limit that we have discussed so far.

To highlight the topological Anderson insulator feature we have also established a conductance map (see Fig. 8), showing the evolution of distinct topological phases and their boundaries as a function of the disorder strength at a fixed number of layers: $N_z = 3$. In the region of relatively small W ($\lesssim 7$) in Fig. 8 one can recognize two insulating regimes separated by a narrow region of a quantized conductance of $G = 2$ starting at $m_0/m_2 = -1$ and $W = 0$. The left insulating region centered at

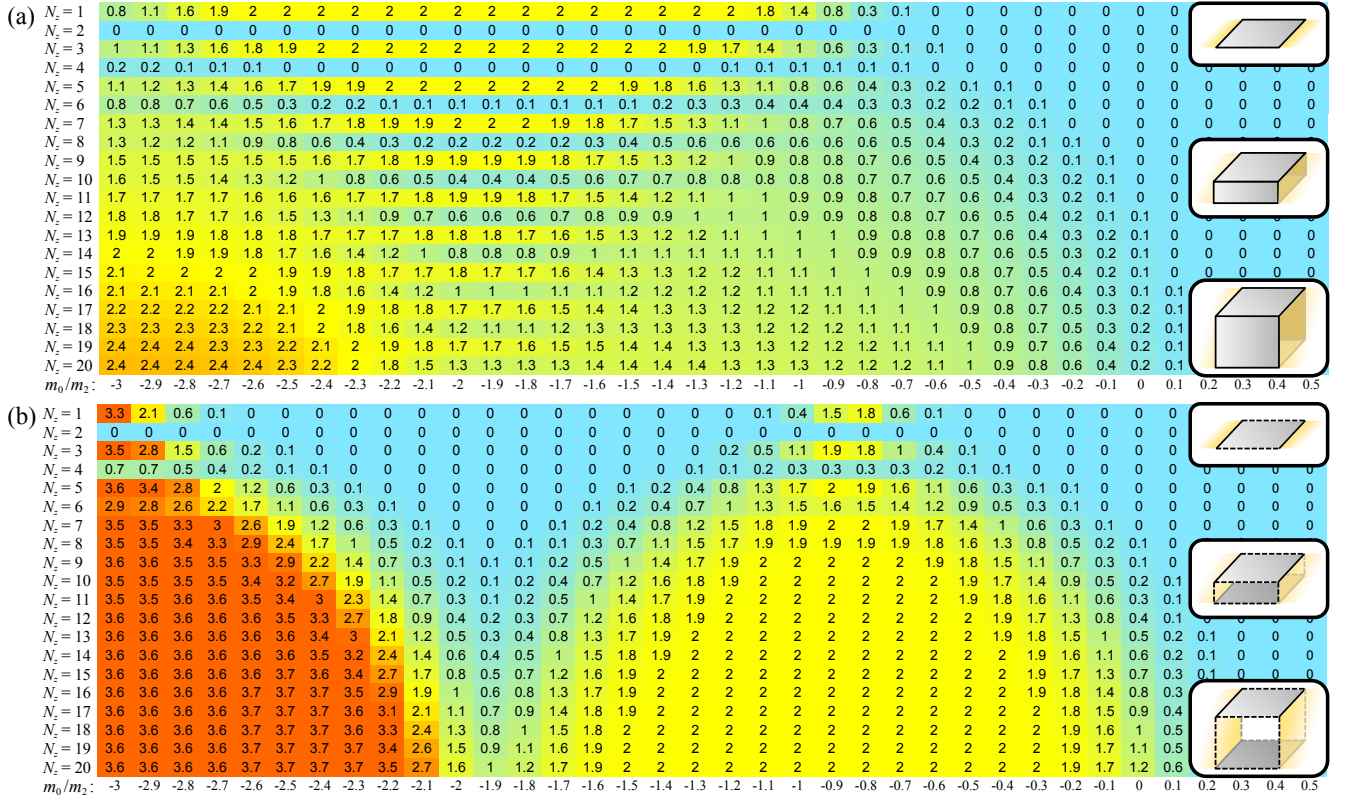


FIG. 7. (Color online) Conductance maps with (a) truncated and (b) periodic boundaries on the y sides. Parameters are the same as in Fig. 2(a) and 2(b) but, here, in the presence of potential disorder ($W = 3$). The average of the conductance over 1000 samples is plotted.

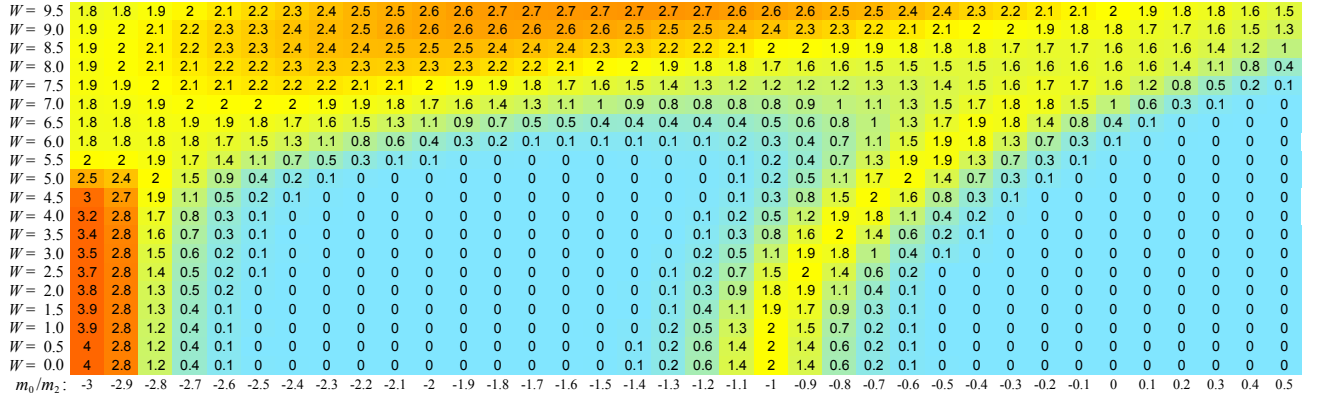


FIG. 8. (Color online) Conductance map for a disordered slab ($N_z = 3$), with varying disorder strength W . Other settings are the same as for Fig. 7(b).

$m_0/m_2 = -2$ at $W = 0$, is the 2D TI (QSHI) phase, while the right region corresponds to the OI phase. The phase boundary with a quantized conductance of $G = 2$ is the 2D version of the Dirac semimetal line studied in Ref. 7. At an m_0/m_2 slightly larger than the location of this Dirac semimetal line, a system in the OI phase is converted to a QSHI upon the addition of disorder (the topological Anderson insulator behavior). At $W \gtrsim 7$ the two insulating phases are both overwhelmed by a diffusive metal phase, a region of large and nonquantized con-

ductance. For the strongly disordered regime $W \gtrsim 15$, the system re-enters the OI (Anderson insulator) phase. These features are most reminiscent of a similar phase diagram obtained earlier for a purely 2D system of the same class AII symmetry,⁴⁵ based on calculation of the localization length. In the structure of the phase diagram shown in Fig. 8, the existence of a diffusive metal phase is characteristic of systems of class AII symmetry. Here, the initial 2D model, the $N_z = 1$ case of Eq. (5) with on-site disorder, belongs to class A, while stacking

more than two layers converts the system to class AII. In contrast to this, only in the addition of Rashba-type spin-orbit coupling in the 2D setup, the system is converted to a model of class AII symmetry in Ref. 45. The setup of the present nanofilm construction is much simpler, and it is an alternative way to realize a class AII QSH system without assuming an s_z nonconserving term.

VI. CONCLUSIONS

We have studied the dimensional crossover of TI nanofilms, focusing on the two types of perfect conduction: surface conduction and edge conduction. Our new conjecture on the two conduction regimes serves as a guideline to interpolate 2D and 3D limits. Based on this conjecture, the simple picture “(QSH) $^{N_z} \simeq$ WTI” has been questioned. Stacking QSH insulators, i.e., “(QSH) N_z ”, does not necessarily lead to the expected WTI (001) state, but to a WTI with other indices or even to an STI as well. For the weak interlayer coupling case $m_{2z} \ll m_{2\parallel}$, 2D QSH and 3D WTI (001) states are indeed linked by an edge conduction regime, but upon approaching the strong interlayer coupling limit $m_{2z} = m_{2\parallel}$, the edge-conduction regimes in a large number of layers are replaced by surface-conduction regimes corresponding to STI or WTI (111) states.

In the regime of small t_z , transport properties in TI nanofilms become rather erratic, reflecting the complicated phase diagram of 2D \mathbb{Z}_2 indices. In the second part of the paper, we have revealed the topological properties of TI thin films (systems with finite thickness and infinite area) as effective 2D systems. We have investigated the 2D \mathbb{Z}_2 phase diagram by direct calculation of the \mathbb{Z}_2 indices and analytical derivation of the locus of the phase boundary for an arbitrary number of layers. The phase diagram implies that a simple even/odd feature with respect to the number of stacked QSH layers sometimes fails. Furthermore, stacked layers of nontopological insulators can enter an emergent 2D topological phase. From the bulk point of view, such an emergent topological phase can also be explained by the inversion of the hybridization gap of pseudogapless surface states.

The strong point of our analysis is that by studying the 2D and 3D topological signatures on an equal footing for different film thicknesses, we could follow precisely how the system evolves from the 2D limit to the 3D limit. Last but not least, the employed method is also valid in the presence of disorder. We have shown that our results are stable against disorder unless the bulk band gap closes.^{6,7} They are also robust against a change in E as long as E is inside the bulk gap, although in this paper, the calculation has been performed for $E = 0$. Here, we assumed a square film geometry ($L_x = L_y$). In the case of a rectangular film ($L_x \gg L_y$), perfect conduction along the x direction will be easier to observe.

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Appendix A: Determination of the phase boundaries in thin films

Diagonalization of the thin-film Hamiltonian, Eq. (5), is not straightforward in general. The gap closing relevant to the topological phase transition occurs only at the four inversion and time-reversal symmetric points Γ_i : (0, 0), (π , 0), (0, π), (π , π). At these points, the Hamiltonian is reduced to

$$H_{\text{film}}(\Gamma_i) = 1_{N_z} \otimes (m_{2D}^{(\Gamma_i)} \beta) + H_z, \quad (\text{A1})$$

where H_z is Eq. (7) and $m_{2D}^{(\Gamma_i)}$ are Eq. (23). Applying β in Eq. (A1) from the left-hand side,

$$\beta H_{\text{film}}(\Gamma_i) = m_{2D}^{(\Gamma_i)} 1_{4N_z} - \begin{pmatrix} 0 & \eta_+ & \ddots & \\ \eta_- & \ddots & \ddots & \\ & \ddots & \ddots & \eta_+ \\ & & \eta_- & 0 \end{pmatrix}, \quad (\text{A2})$$

where

$$\eta_{\pm} = \frac{m_{2z}}{2} 1_4 \pm i \frac{t_z}{2} \beta \alpha_z. \quad (\text{A3})$$

Note that η_{\pm} are nonunitary matrices and

$$\eta_- \eta_+ = \eta_+ \eta_- = \kappa 1_4, \quad (\text{A4})$$

where

$$\kappa = \left(\frac{m_{2z}}{2} \right)^2 - \left(\frac{t_z}{2} \right)^2. \quad (\text{A5})$$

To find the gapless points, we assume that $H_{\text{film}} \mathbf{u} = 0$ for an appropriate state vector \mathbf{u} . Then Eq. (A2) is considered to be a generalized eigenvalue problem for a non-Hermitian matrix:

$$\begin{pmatrix} 0 & \eta_+ & \ddots & \\ \eta_- & \ddots & \ddots & \\ & \ddots & \ddots & \eta_+ \\ & & \eta_- & 0 \end{pmatrix} \mathbf{u} = m_{2D}^{(\Gamma_i)} \mathbf{u}. \quad (\text{A6})$$

Here we assume a right eigenvector of the form

$$\mathbf{u}_n = C \begin{pmatrix} \psi_{1,n} \chi_{\pm} \\ \psi_{2,n} \chi_{\pm} \\ \vdots \\ \psi_{N_z,n} \chi_{\pm} \end{pmatrix}, \quad \psi_{j,n} = c_j \sin(j k_z^{(n)}), \quad (\text{A7})$$

where C is the normalization factor and χ_{\pm} is an eigenspinor of η_{-} with eigenvalue $\epsilon_{\pm}\sqrt{\kappa} = \frac{m_{2z}}{2} \pm \frac{t_z}{2}$,

$$\frac{\eta_{-}}{\sqrt{\kappa}}\chi_{\pm} = \epsilon_{\pm}\chi_{\pm}. \quad (\text{A8})$$

(Note χ_{+} and χ_{-} correspond to the top and bottom surface eigenstates, respectively.) Then the scalar coefficients c_j follow the relation,

$$\lambda_n c_j \sin(jk_z^{(n)})\chi_{\pm} = c_{j-1} \sin((j-1)k_z^{(n)})\eta_{-}\chi_{\pm} + c_{j+1} \sin((j+1)k_z^{(n)})\eta_{+}\chi_{\pm}, \quad (\text{A9})$$

with λ_n the eigenvalue of Eq. (A6). Using Eq. (A4), equation (A9) can be simplified by applying η_{-} from the left hand side, as

$$\lambda_n c_j \epsilon_{\pm} \sqrt{\kappa} \sin(jk_z^{(n)}) = c_{j-1} \epsilon_{\pm}^2 \sin((j-1)k_z^{(n)}) + c_{j+1} \sin((j+1)k_z^{(n)}). \quad (\text{A10})$$

One can find the solution of Eq. (A10),

$$c_j = \epsilon_{\pm}^{j-1}, \quad (\text{A11})$$

with the normalization factor,

$$\frac{1}{C^2} = \sum_{j=1}^{N_z} \epsilon_{\pm}^{2(j-1)} \sin^2(jk_z^{(n)}), \quad (\text{A12})$$

and the eigenvalues

$$\lambda_n = 2\sqrt{\kappa} \cos k_z^{(n)}. \quad (\text{A13})$$

Therefore the gap of the film closes at $4N_z$ points [see Eq. (31)] on the complex plane, where $m_{2D}^{(\Gamma_i)} = \lambda_n$.

We mention that for $t_z^2 < m_{2z}^2$, the emergent 2D topological phases appear inside the ellipse in the (m_0, t_z) space (see also Fig. 6),

$$\left(\frac{m_0 - m_{0c(N_z=1)}^{\Gamma_i}}{\cos k_z^{(n=1)}} \right)^2 + t_z^2 = m_{2z}^2, \quad (\text{A14})$$

and this corresponds to the parameter region where the damped oscillating behavior of the surface wave function emerges in the semi-infinite model [Eq. (54) in Ref. 33].

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